2,3,4-Trifluorophenol, methyl ether

Inchi: InChI=1S/C7H5F3O/c1-11-5-3-2-4(8)6(9)7(5)10/h2-3H,1H3
InchiKey: LIVNSQZJDRPZKP-UHFFFAOYSA-N
Formula: C7H5F3O
SMILES: COc1ccc(F)c(F)c1F
Mol. weight [g/mol]: 162.11

Physical Properties

Property code	Value	Unit	Source
gf	-597.85	kJ/mol	Joback Method
hf	-706.24	kJ/mol	Joback Method
hfus	17.19	kJ/mol	Joback Method
hvap	35.40	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.113		Crippen Method
mcvol	96.910	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
rinpol	962.10		NIST Webbook
tb	421.41	K	Joback Method
tc	603.75	K	Joback Method
tf	256.63	K	Joback Method
vc	0.392	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.57	J/mol×K	421.41	Joback Method
cpg	195.64	J/mol×K	451.80	Joback Method
cpg	203.45	J/mol×K	482.19	Joback Method
cpg	210.98	J/mol×K	512.58	Joback Method
cpg	218.23	J/mol×K	542.97	Joback Method
cpg	225.21	J/mol×K	573.36	Joback Method
cpg	231.91	J/mol×K	603.75	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352616&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume